

WHAT IS CLAIMED IS:

1. A method for improving an electron density map representing a crystal structure comprising:

(a) obtaining by x-ray diffraction observed structure factor amplitudes for a plurality of reflections from the crystal structure;

5 (b) selecting a starting set of crystallographic phases to combine with the observed structure factor amplitudes to form a first set of structure factors;

(c) deriving a first electron density map from the first set of structure factors;

10 (d) identifying features of the first electron density map to obtain expected distributions of electron density;

(e) making a comparison between the first electron density map and the expected distribution of electron density;

(f) estimating how changes in the crystallographic phase of a reflection k affect the comparison;

15 (g) establishing crystallographic phase probability distributions from the comparisons for the possible crystallographic phases of reflection k ;

(h) repeating steps (c) through (g) as k is indexed through all of the plurality of reflections;

20 (i) deriving an updated electron density map using crystallographic phases determined to be most probable from the crystallographic phase probability distributions for each one of the reflections; and

(j) repeating steps (d) through (i) to obtain a final set of crystallographic phases with minimum bias from known electron density maps.

2. The method of Claim 1, wherein identifying features of the electron density map includes making probability estimates of whether each point in the map is located in a solvent region or a crystal structure region.

3. The method of Claim 1, wherein identifying features of the election density map includes estimates of whether the electron density at each point in the map is related by non-crystallographic symmetry to electron density at another point in the map.

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- combining the weighted structure factors with the observed structure factors for deriving the first electron density map.